Coarse-grained model for water and water-protein interfaces.

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We study, by Monte Carlo simulations, a coarse-grained model for nanoconfined water that includes many-body interactions associated to water cooperativity, originally introduced by Franzese and Stanley (FS) [1]. The FS model is computationally efficient [2] and allows us to equilibrate water at extreme low temperatures *T* in a wide range of pressures *P* [3,4]. Moreover, it can be easily extended to include proteins, so we can analyze the behavior of the water-protein interface and how the solvent affects the protein configuration [5,6]. Here, we focus on the phase diagram of the FS model, showing that it reproduces, at least qualitatively, the experimental water phase diagram both in confinement and in bulk [7], a prerequisite for using it as a proper solvent in protein solutions. Our results compare well with atomistic simulations and show, for both confined (Figure 1) and bulk water, the presence of a low-density liquid and a high-density liquid water phases, separated by a liquid-liquid phase transition ending in a liquid-liquid critical point. Our results clarify fundamental properties of hydration and bulk water and are potentially useful for better understanding the effects of *T* and *P* on nano-bio-interactions among proteins and other species or interfaces.

References

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Figures

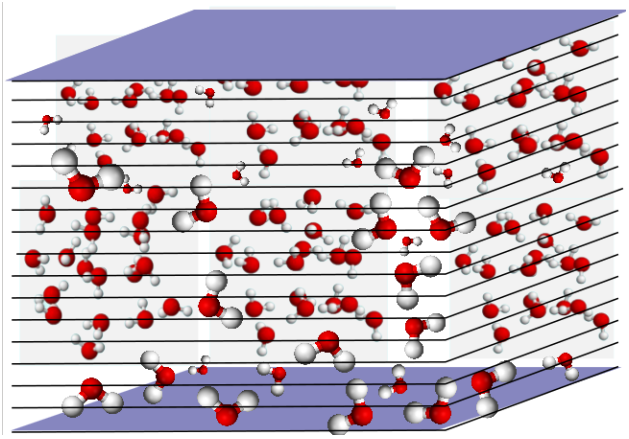

Figure 1. Schematic representation of water multilayers under nanoconfinement. We consider a system of 20 layers corresponding to a separation between walls of 6 nm.